Electronic Supplementary Information (ESI)

High Thermoelectric Performance of Two-Dimensional SiPGaS/As Heterostructures

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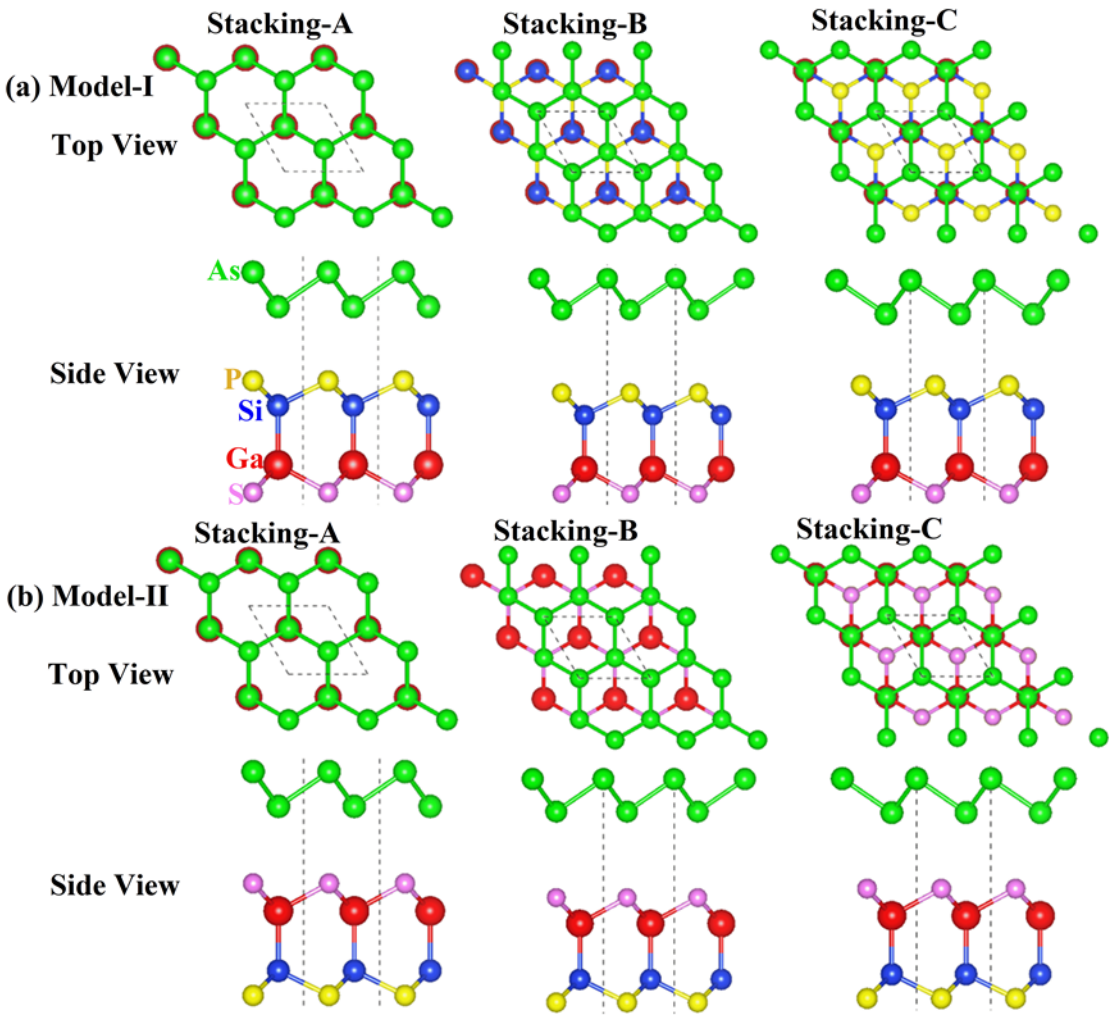

Fig. S1. Possible stackings and top/side views of model-I (a) and model-II (b). Black vertical lines represent the unit cell.

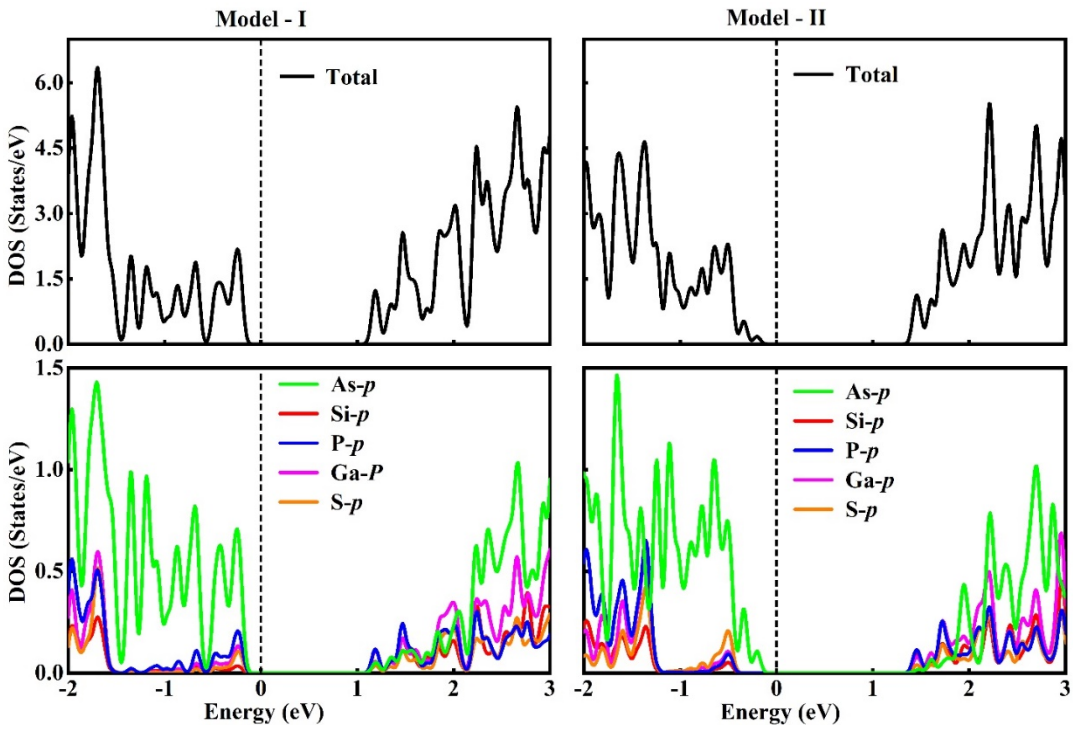

Fig. S2. Calculated total (TDOS) and partial density of states (PDOS) of model-I and model-II using HSE06 functional.

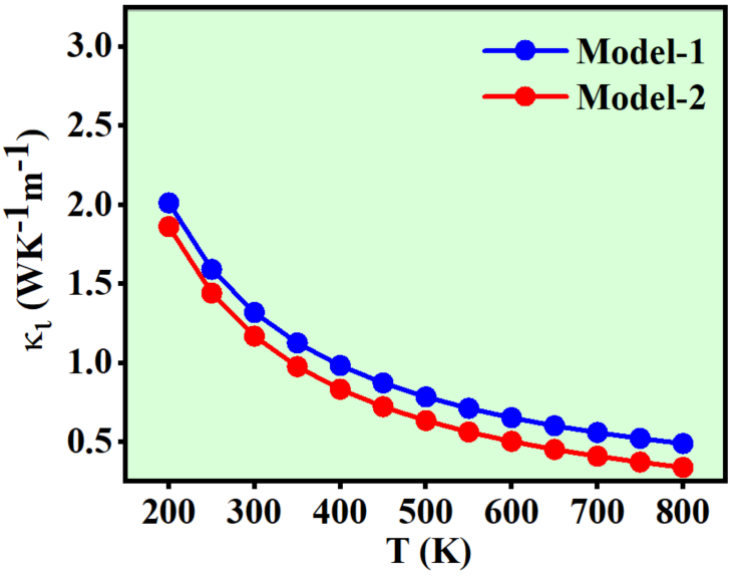

Fig. S3. Calculated lattice thermal conductivity of model-I and model-II at biaxial 4% tensile strain.

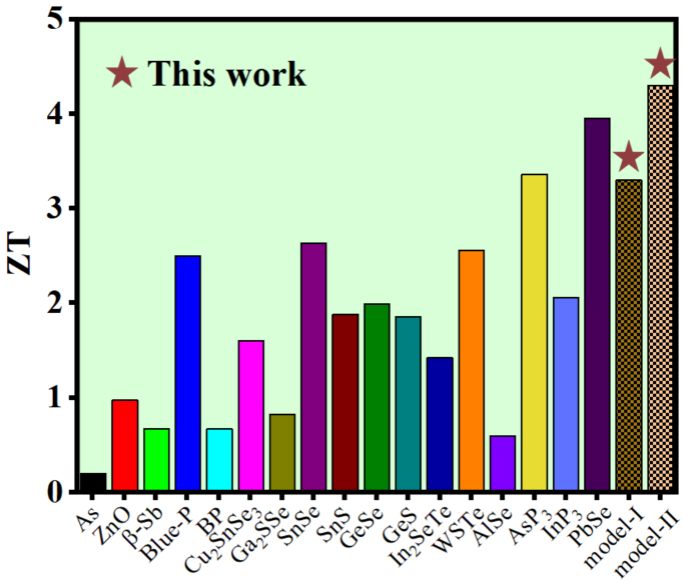

Fig. S4. Comparison of ZT of model-I and model-II with reported monolayers.

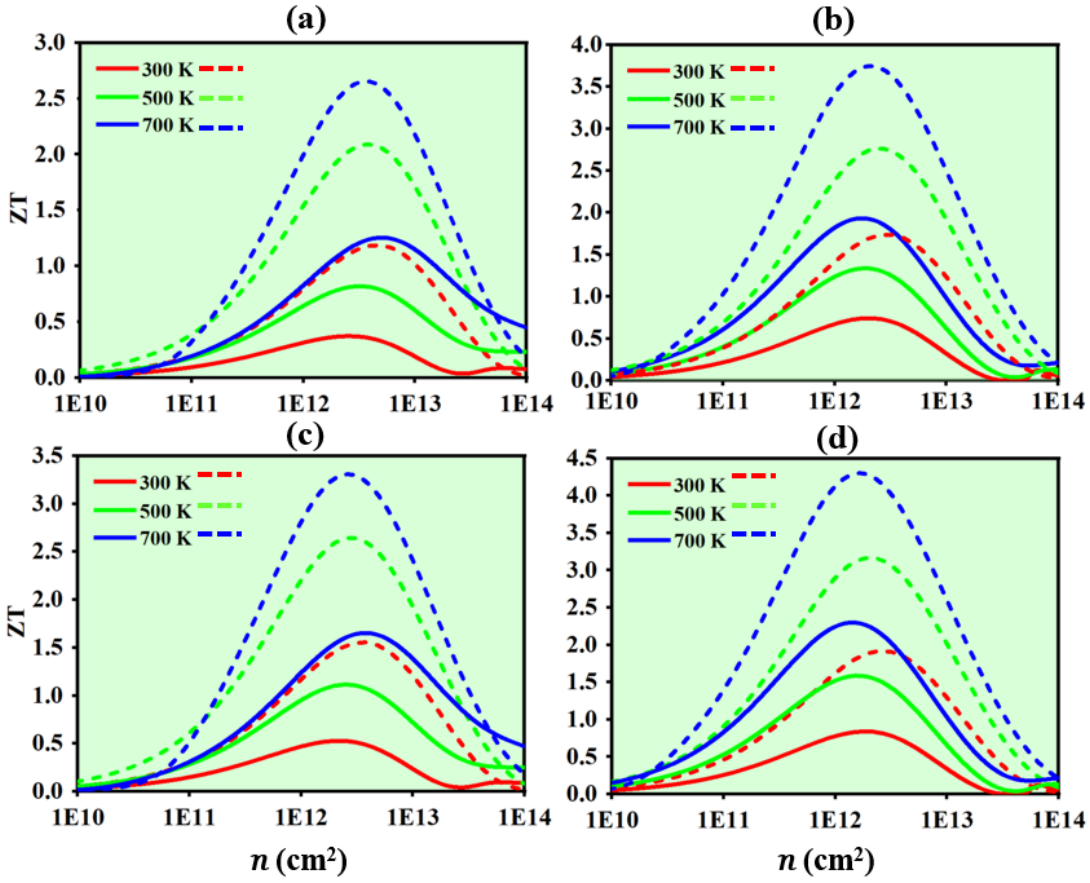

Fig. S5. ZT as a function of carrier concentration. (a) Unstrained and (c) strained model-I, (b) Unstrained and (d) strained model-II at different temperatures. The solid and dashed line represent p- and n-type doping, respectively.

Table S1. Binding energy E_i (eV) for different stacking (i=a, b, c), inter-layer distance d_o (Å), lattice parameters a (Å), bond lengths d_{As-As}, d_{Si-P}, d_{Si-Ga}, d_{S-Ga} (Å), work function (Φ/eV), band gaps E_g (eV) using PBE and HSE functionals for both Model-I and Model-II heterostructures. Conduction band minimum (CBM) and valence band maximum (VBM)

Heterostructures	Model-I	Model-II
E_a	-1.57	-1.54
d_o	3.65	3.73
E_b	-1.48	-1.47
d_o	3.73	3.73
E_c	-1.56	-1.53
d_o	3.61	3.75
Φ	5.50	5.69
CBM	-4.33	-4.26
VBM	-5.71	-5.90
a	3.55	3.55
d_{As-As}	2.49	2.49
d_{Si-P}	2.28	2.28
d_{Si-Ga}	2.42	2.42
d_{S-Ga}	2.34	2.34
E_g (PBE)	0.80	1.00
E_g (HSE)	1.39	1.64

Table S2. Deformation potential constants Ei (eV), in-plane stiffness C_{2D} (Nm^{-1}), carrier effective masses m* (m_e) and carrier mobilityμ ($cm^2V^{-1}S^{-1}$) for e and h carrier respectively.

Models	Carrier	E_i	C_{2D}	m^*	μ
Model-I	e	-3.86	159.43	0.69	3.20×10^2
	h	-5.60	159.43	0.70	1.47×10^2
Model-II	e	-3.19	159.93	0.71	4.44×10^2
	h	-1.51	159.93	0.63	2.51×10^2